Signature inversion – manifestation of drift of the rotational axis in triaxial nuclei

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Abstract

A possible scheme of realizing shell model calculations for heavy nuclei is based on a deformed basis and the projection technique. Here we present a new development for odd-odd nuclei, in which one starts with triaxially-deformed multi-quasi-particle configurations, builds the shell-model space through exact three-dimensional angular-momentum-projection, and diagonalizes a two-body Hamiltonian in this space. The model enables us to study the old problem of signature inversion from a different view. With an excellent reproduction of the experimental data in the mass-130 region, the results tend to interpret the phenomenon as a manifestation of dynamical drift of the rotational axis with presence of axial asymmetry in these nuclei.

Key words: shell model, angular momentum projection, triaxial deformation, signature inversion
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There have been many unusual and interesting features discovered in the nuclear high-spin rotational spectra. To describe them, it is not feasible to apply the conventional shell models constructed in a spherical basis. Description of heavy, deformed nuclei has therefore relied mainly on the mean-field approximations [1], or sometimes on the phenomenological particle-rotor model [2]. However, there has been an increasing number of compelling evidences indicating that correlations beyond the mean-field level are important and a proper quantum-mechanical treatment for nuclear states is necessary. It is thus important to develop alternative types of nuclear structure model that can incorporate the missing many-body correlations and make shell-model calculations possible also for heavy nuclei.

This Letter reports on a new theoretical development for doubly-odd systems, in line with the effort of developing shell models using deformed bases [3,4,5,6]. The present model employs a triaxially deformed (or γ deformed) basis, constructs the model space by including multi-quasi-particle (qp) states (up to 6-qp), and performs exact three-dimensional angular momentum projection. A two-body Hamiltonian is then diagonalized in this space. The idea has been applied so far only in the simplest case with a triaxially-deformed qp vacuum state [6,7,8]. The current work is the first attempt to realize the triaxial projected shell model idea in a realistic situation with a configuration mixing in a multi-qp model space. As the first application, we address the long-standing question on signature inversion, a phenomenon which has been widely observed in nuclear rotational spectrum but not been convincingly explained.

This phenomenon has been suggested to relate to one of the intrinsic symmetries in nuclei, which corresponds to "deformation invariance" [9]. Due to this property, rotational energies $E(I)$ (I: total spin of a state) of a high-j band can be split into two branches with $\Delta I = 2$, classified by the signature quantum number, α [2]. As a rule, the energetically favored sequence has $I = j \pmod 2$ and unfavored one $I = j + 1 \pmod 2$, with j being, for a doubly-odd system, the sum of the angular momenta that the last neutron and the last proton carry. A more general signature rule from a quantum-mechanical derivation was given in Ref. [10]. The critical observation for signature inversion [11] is that at low spins, the energetically unfavored sequence is abnormally shifted downwards, exhibiting, in an $E(I) - E(I-1)$ plot, a reversed zigzag phase to what the signature rule predicts (see Fig. 1 below). Only beyond a moderate spin $I_{\rm rev}$, which is called reversion spin [12], is the normal zigzag phase restored. The cause of signature inversion has been a major research subject for many years.

As the first attempt of explanation, triaxiality in the nuclear shape was suggested to be the primary reason [13]. With presence of γ deformation ($0^\circ \le \gamma \le 60^\circ$), the lengths of the two principal axes, the x- and y-axis, are different. If one assumes as usual that the moment of inertia has the same shape dependence as that of irrotational flow, a nucleus prefers to rotate around its intermediate-length principal axis, the y-axis [2]. However, a nucleus with reversed zigzag phase requires a rotation around its shortest principal axis, the x-axis. To describe signature inversion, one had to introduce [14,15] the concept of γ-reversed moment-of-inertia in which one changes the rotation axis by hand. Unsatisfied with this kind of approach, Tajima [16] suggested that other ingredients in addition to triaxiality have to be taken into account. The most popular one discussed in the literature is the neutron-proton interaction [17].

We show that the phenomenon can be naturally described by shell-model-type calculations without invoking unusual assumptions. We first outline our

model. The wave-function can be written as

$$|\Psi^{\sigma}_{IM}\rangle = \sum_{K\kappa} f^{\sigma}_{IK_\kappa}\, \hat{P}^{I}_{MK}\, |\Phi_\kappa\rangle \,, \tag{1}$$

in which the projected multi-qp states span the shell model space. In Eq. (1), $|\Phi_\kappa\rangle$ represents a set of 2-, 4-, and 6-qp states associated with the triaxially deformed qp vacuum $|0\rangle$

$$\begin{aligned}&\{\alpha^\dagger_{\nu_1}\alpha^\dagger_{\pi_1}|0\rangle\,, \quad \alpha^\dagger_{\nu_1}\alpha^\dagger_{\nu_2}\alpha^\dagger_{\nu_3}\alpha^\dagger_{\pi_1}|0\rangle\,, \quad \alpha^\dagger_{\nu_1}\alpha^\dagger_{\pi_1}\alpha^\dagger_{\pi_2}\alpha^\dagger_{\pi_3}|0\rangle\,,\\ &\alpha^\dagger_{\nu_1}\alpha^\dagger_{\nu_2}\alpha^\dagger_{\nu_3}\alpha^\dagger_{\pi_1}\alpha^\dagger_{\pi_2}\alpha^\dagger_{\pi_3}|0\rangle\}.\end{aligned} \tag{2}$$

The dimension in Eq. (1) is $(2I+1)\times n(\kappa)$, where $n(\kappa)$ is the number of configurations and is typically in the order of 10^2. $\hat{P}^I_{MK}$ is the three-dimensional angular-momentum-projection operator [1]

$$\hat{P}^{I}_{MK} = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I}_{MK}(\Omega)\, \hat{R}(\Omega), \tag{3}$$

and σ in Eq. (1) specifies the states with the same angular momentum I.

The triaxially deformed qp states are generated by the Nilsson Hamiltonian

$$\hat{H}_N = \hat{H}_0 - \frac{2}{3}\hbar\omega\epsilon_2\left(\cos\gamma\hat{Q}_0 - \sin\gamma\frac{\hat{Q}_{+2}+\hat{Q}_{-2}}{\sqrt{2}}\right), \tag{4}$$

where the parameters ϵ_2 and γ describe quadrupole deformation and triaxial deformation, respectively. Three major shells (N = 3, 4, 5) are considered each for neutrons and protons. Paring correlations are included by a subsequent BCS calculation for the Nilsson states.

The Hamiltonian consists of a set of separable forces

$$\hat{H} = \hat{H}_0 - \frac{1}{2}\chi\sum_\mu \hat{Q}^\dagger_\mu\hat{Q}_\mu - G_M\hat{P}^\dagger\hat{P} - G_Q\sum_\mu \hat{P}^\dagger_\mu\hat{P}_\mu. \tag{5}$$

In Eq. (5), $\hat{H}_0$ is the spherical single-particle Hamiltonian, which contains a proper spin-orbit force [18]. The second term is quadrupole-quadrupole (QQ) interaction that includes the nn, pp, and np components. The QQ interaction strength χ is determined in such a way that it has a self-consistent relation with the quadrupole deformation [3]. The third term in Eq. (5) is monopole pairing, whose strength G_M (in MeV) is of the standard form G/A, with $G = 19.6$ for neutrons and 17.2 for protons, which approximately reproduces

Table 1
Quadrupole deformation ϵ_2 and triaxial deformation γ employed in the calculation.

Nucleus	118	120	122	124	126	128	130
ϵ_2	0.30	0.29	0.26	0.26	0.21	0.20	0.19
γ	30°	30°	31°	31°	35°	37°	39°

the observed odd-even mass differences in this mass region. The last term is quadrupole pairing, with the strength G_Q being proportional to G_M, the proportionality constant being fixed as usual to be 0.16 for all nuclei considered in this paper. In our model, wherever the quadrupole operator appears, we use the dimensionless quadrupole operator (defined in Section 2.4 of Ref. [3]). We emphasize that no new terms in the Hamiltonian are added and no interaction strengths are individually adjusted in the present work to reproduce data.

To observe a sizable effect of signature, one important condition is that nucleons near the Fermi levels occupy the lower part of high-j shells having smaller K-components. A recent summary for the observed $\pi h_{11/2} \nu h_{11/2}$ bands in the mass-130 region has been given by Hartley *et al.* [12]. Note that experimental deduction of spins for bands in doubly-odd nuclei is often difficult. We apply the spin values suggested by Liu *et al.* [19] to each of the bands if spin is not firmly determined. The normal signature rule for these bands is that the energetically favored states have odd-integer spins denoted by $\alpha = 1$ and the unfavored ones have even-integer spins denoted by $\alpha = 0$. However, a systematic violation of this rule has been observed in the lower spin states. In Ref. [10], a mechanism for explaining the observed signature inversion data in some rare earth nuclei was proposed, which employed the projected shell model [3] based on an axially deformed basis. This mechanism involved a crossing of two rotational bands that have mutually opposite signature dependence. However, early studies [20] showed that it is not possible for this mechanism to explain the data in the present study because the condition of having bands near the Fermi levels with mutually opposite signature dependence does not appear here.

The present calculations are performed for doubly-odd nuclei $^{118-130}$Cs. In Table I, we list the deformation parameters used for basis construction. The quadrupole deformation parameters ϵ_2 are consistent with those obtained from the TRS calculations. The γ parameters are adjusted to describe not only the bands discussed in this paper, but also other observables (see discussions below). Our results are compared with available data in Fig. 1 in the form of energy difference between states of the two signature sequences. As one can see, an excellent agreement has been achieved. With an increasing neutron number, the trend of decreasing signature splitting, i.e. decreasing zigzag amplitude, has been reproduced. What is also correctly described is the increasing trend

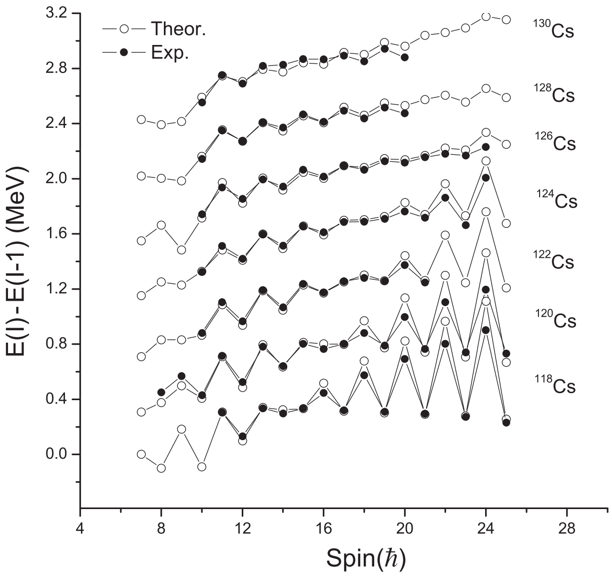

Fig. 1. Comparison of calculated energies with data for the $\pi h_{11/2}\nu h_{11/2}$ bands in $^{118-130}$Cs. Note the increasing trend in the reversion spin: 14.5 for ^{118}Cs, 16.5 for ^{120}Cs, 17.5 for ^{122}Cs, 18.5 for ^{124}Cs, 20.5 for ^{126}Cs, 21.5 for ^{128}Cs (prediction), and 22.5 for ^{130}Cs (prediction). Note also that the bands are shifted vertically by $(A-118) \times 0.2$ MeV where A is mass number.

of $I_{\rm rev}$ as neutron number increases.

Now we investigate how signature inversion occurs in our theory. We first study the effect of triaxiality. It has been known that γ is a relevant degree of freedom in this mass region, and the nuclei are either γ-deformed or γ-soft. For example, a stable γ deformation is required in the discussion of chiral doublet bands [21]. In Fig. 2, we take ^{124}Cs as an example to present the calculated bands as a function of γ. Namely, we allow γ in Eq. (4) to vary, while all other parameters are fixed as those in the ^{124}Cs results in Fig. 1. It is observed that the splitting between the two signature sequences is strongly dependent on γ. With $\gamma = 0$, no clear signature splitting can be seen for the lower spin states. This explains why one could not describe the data when an axially deformed basis is used [20]. An increasing trend of splitting is obtained as γ increases, with the maximum splitting appearing with $\gamma = 30°$. This is the γ value corresponding to the maximal triaxiality, after which the splitting shows a decreasing trend. Note that signature splitting and inversion of the zigzag phase are visible only when γ is sufficiently large ($\geq 10°$). Note also that the reversion spin $I_{\rm rev}$ does not change with γ.

In a shell-model calculation, wavefunctions contain all information about the evolution of a system. We demonstrate that signature inversion and the zigzag phase restoration are the consequence of a dynamical process in which the rotational axis drifts from the x- to the y-direction of the principal axis as a triaxial odd-odd nucleus is rotating. To see this, we have calculated expectation values

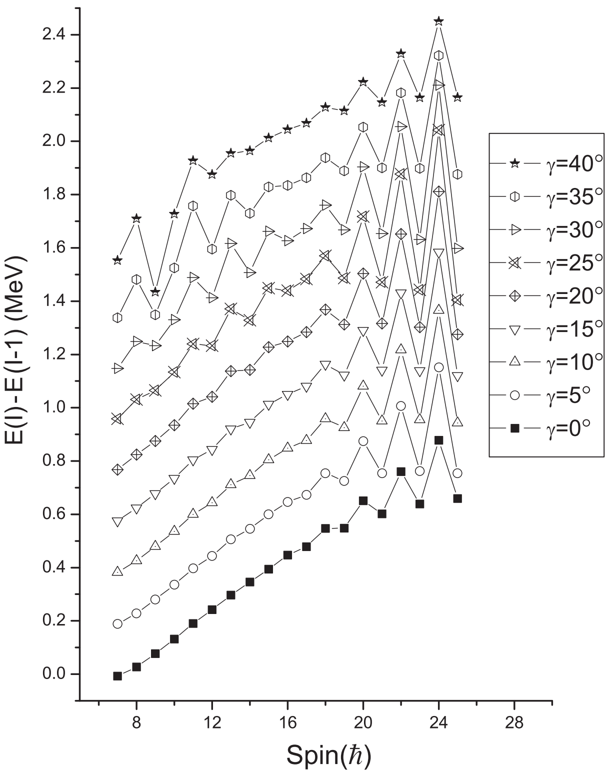

Fig. 2. Calculated 2-qp $\pi h_{11/2}\nu h_{11/2}$ bands in ^{124}Cs with different triaxiality in the basis. Note that the bands are shifted vertically by $\gamma/25°$ MeV.

of the three components of angular-momentum operator, $\hat{I}_i^2$ ($i = x, y$ and z). We plot I_i^2 in Fig. 3 as functions of spin. It is seen that in the entire spin range, I_z^2 takes very small, near-constant values, indicating that the system does not rotate around the z-axis. Near-zero I_y^2 is also seen until $I = 11$; however, it begins to climb up drastically after that spin. In contrast, I_x^2 increases gradually at low spins until $I = 16$, oscillates afterwards between odd and even spins, and then quickly decreases beyond $I = 24$. We thus end up with the following picture: At low spins, the system rotates around the x-axis. Starting from $I = 12$, the rotational axis begins to drift toward the y-direction with a angle in the x-y plane determined by I_x^2 and I_y^2. For example, at $I = 18$ where $I_x^2 \approx I_y^2$, the angle takes 45°. With increasing spin, I_y^2 quickly dominates and the rotation eventually aligns completely with the y-axis. We conclude that roughly in the spin interval $I = 12 - 24$, the rotational axis completes a drift from x-axis to y-axis, and in this process, the reversed zigzag phase is restored. $I_{\rm rev}$ is just the spin where the I_x^2 and I_y^2 curves (taken average values of the odd and even spins) cross.

The effect of neutron-proton interaction on the signature inversion has been extensively discussed [17]. Recently, Xu *et al.* have proposed [22] that quadrupole-pairing force may also have an important contribution. We study the effect of neutron-proton interaction in the QQ channel by changing the n-p interaction strength $\chi_{\rm np}$ in Eq. (5). In Fig. 4(a), we present calculations with different $\chi_{\rm np}$

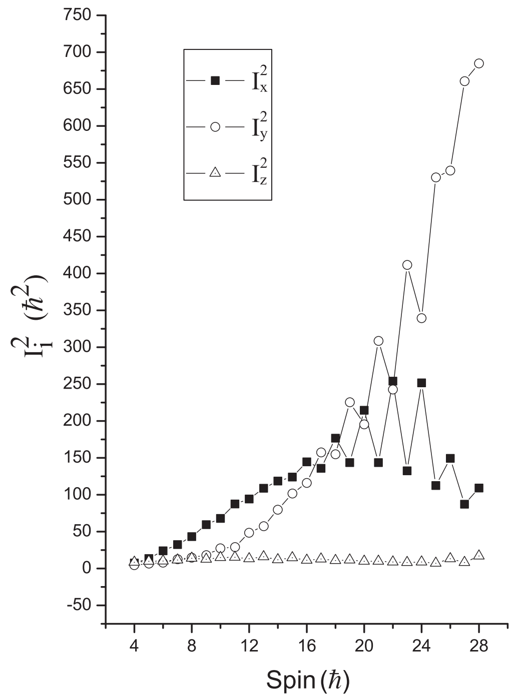

Fig. 3. Calculated expectation values of I_x^2, I_y^2 and I_z^2 with the wavefunctions from diagonalization that has reproduced the ^{124}Cs data (see Fig. 1).

by multiplying a factor $F_{\rm np}$ to its original value. Comparing the four sets of calculations, one sees that in the lower spin region they are nearly identical. The four curves in the higher spin region are also very similar with differences only in the splitting amplitude. The main effect caused by this interaction is to shift the reversion spin. For example, with $F_{\rm np} = 0$, $I_{\rm rev} = 15.5$. $I_{\rm rev}$ shifts higher to 16.5 with $F_{\rm np} = 1$, and to 17.5 when $F_{\rm np} = 2$. Similar conclusion also holds for quadrupole-pairing force, as one can see from Fig. 4(b). In the four sets of calculations with different quadrupole-pairing strengths, the difference is only a shift of $I_{\rm rev}$ toward higher spins with an increasing strength. We have thus found that within our model, signature inversion occurs with $F_{\rm np} = 0$ and $G_Q = 0$.

We notice that the values of γ-parameter that account for the experimental data of signature inversion are not always supported by potential energy calculations from mean-field models which in many cases predict small or zero triaxiality [22]. It turns out that the correct accounting of the correlations provided by the angular momentum projection tends to lower the potential energy in the triaxial deformation region [23]. Calculations have shown that such a tendency may be common to all kinds of nuclei [24]. The calculated B(M1)/B(E2) in ^{124}Cs, as shown in Fig. 5, suggest that the γ values in Table I can reproduce not only the energy levels, but also the transitions. We have verified that the same set of parameters can well describe other observables such as the side bands in $^{124-130}$Cs and the Yrast and γ-vibrational states in the neighboring even-even nuclei. These results will be published elsewhere.

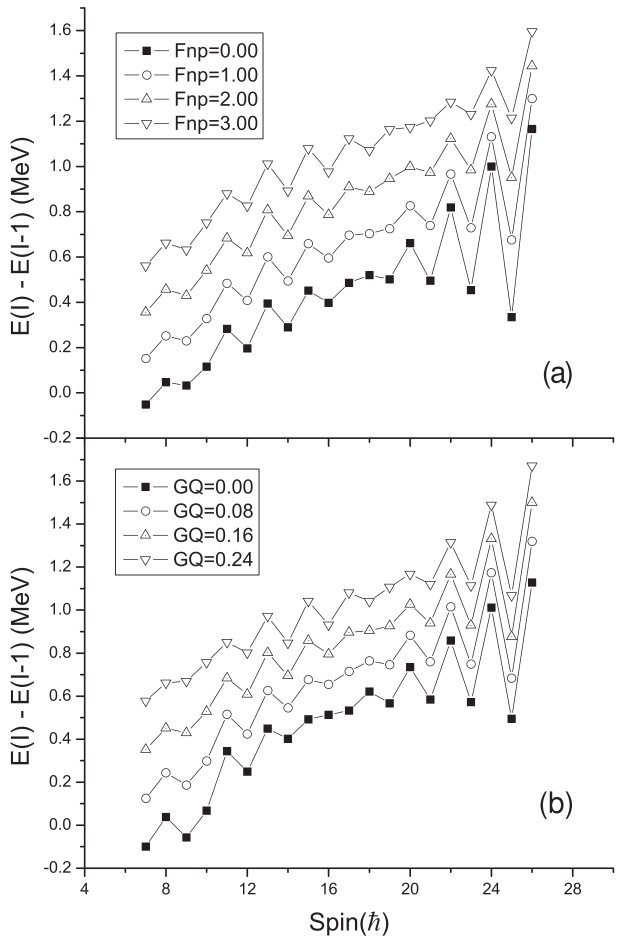

Fig. 4. Calculated $\pi h_{11/2}\nu h_{11/2}$ bands in ^{124}Cs with (a) different $\chi_{\rm np}$, and (b) different G_Q in the Hamiltonian (5). Note that the bands are successively shifted vertically by 0.2 MeV.

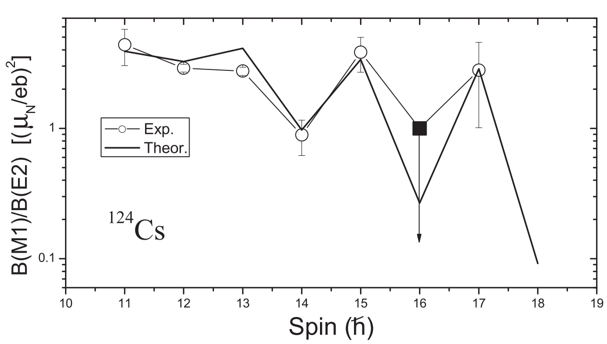

Fig. 5. Comparison of calculated B(M1)/B(E2) with data in ^{124}Cs.

To summarize, the phenomenon of signature inversion has been known for more than two decades. Here, experimental data are reproduced systematically with high accuracy, without the need of invoking any unusual assumptions associated with shape change or with interactions. The key to the success may be the shell-model nature of the method. Our states $|\Psi_{IM}\rangle$ have an advantage over the unprojected state $|0\rangle$ in that the projection treats the states

fully quantum-mechanically by collecting all the energy-degenerate mean-field states associated with the rotational symmetry. This suggests that the effects brought by a quantum-mechanical treatment for a nuclear system should not be overlooked. We have shown that with the triaxial projected shell model in a realistic configuration space, signature inversion data in the mass-130 region can be reproduced nicely with the separable forces in the standard form. The degree of triaxiality in the deformed basis determines the magnitude of signature splitting and the occurrence of signature inversion. The residual interactions, such as the Q_nQ_p and the quadrupole-pairing force, merely modify the position where the reversed zigzag phase is restored. By analyzing the rotational evolution of the components of angular momentum, we have interpreted the phenomenon of signature inversion as a manifestation of the dynamical process in triaxial nuclei, in which the rotational axis drifts from the shortest principal axis to the intermediate one as nuclei are rotating. Discussion of drift of angular momentum axis in one-quasiparticle states was given by Ikeda and Åberg in terms of the particle-rotor model [25].

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